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Table 1S. Comparison of geometries calculated with *ab initio* QC[a] and with FF (MSX and UFF) for $(MeO)_2PS_2^-$.

	tt			*tg*$^+$			*g*$^+$*g*$^+$	
	QC	MSX	UFF	QC	MSX	UFF	QC	MSX	UFF
Bonds (Å)									
C-H	1.084	1.085	1.111	1.084	1.085	1.111	1.084	1.085	1.111
S-P	1.993	1.992	2.162	1.988	1.993	2.162	1.983	1.995	2.159
O-C	1.400	1.403	1.406	1.401	1.404	1.406	1.402	1.405	1.406
P-O	1.634	1.632	1.750	1.640	1.635	1.751	1.647	1.639	1.752
Angles (degrees)									
H-C-H	109.3	109.6	108.6	109.3	109.5	108.6	109.1	109.5	108.6
P-O-C	119.7	119.5	108.3	120.7	120.4	108.2	120.7	121.1	108.3
S-P-O	110.3	110.2	109.7	109.3	110.3	109.6	108.2	110.3	109.7
O-C-H	109.7	109.4	110.3	109.7	109.4	110.3	109.9	109.4	110.3
O-P-O	93.6	93.7	104.2	96.3	93.5	105.5	99.5	93.3	105.9
S-P-S	119.3	119.5	113.4	120.7	120.7	112.8	122.2	122.1	112.0
C-O-P-O	180/180	180/180	180/180	179.3/65.5	179.0/67.7	180.0/56.2	67.9/67.9	70.2/70.2	63.3/63.3
Energy (kcal/mol)									
	0[b]	0	0	0.17	0.20	−2.23	0.62	0.70	−2.41

[a]HF/LAV3P***.

[b]Total energy: −255.24750 Hartree.

Table 2S. Effect of basis sets on Zn-DTP coordination for $Zn(SH)[(MeO)_2PS_2]$ from HF calculations. Each column lists the relative energies (kcal/mol) for a given level of calculation. LAV3P and LANL1DZ use effective core potentials while MSV is all electron. *** indicates polarization functions on all atoms (the most reliable). No stars indicates no polarization functions. See Section II.A.

Basis Set	MSV***	LAV3P***	LAV3P**	MSV	LAV3P	LAN1DZ
Basis Fns.	195	171	146	129	105	100
SS[a]	0.0[b]	0.0[c]	0.0[d]	0.0[e]	0.0[f]	0.0[g]
OS[a]	10.5	9.7	2.6	-7.2	-9.1	-8.3
OO[a]	28.0	27.5	15.0	-8.3	-9.2	-7.7

[a]This indicates to which atoms of DTP the zinc atom binds.

[b]Total energy: −3536.78677 Hartree.

[c]Total energy: −329.31395 Hartree.

[d]Total energy: −329.11287 Hartree.

[e]Total energy: −3536.4363 Hartree.

[f]Total energy: −328.98707 Hartree.

[g]Total energy: −329.02699 Hartree.

Table 3S. *Ab initio* results for Zn(SH)[$(MeO)_2PS_2$] from HF/LAV3P*** calculations.

	tt	tg^+	g^+g^+
Bonds (Å)			
C-H	1.080	1.080	1.081
S-P	2.033	2.027	2.022
O-C	1.424	1.425	1.426
P-O	1.584	1.588	1.594
Zn-S_{DTP}	2.438	2.442	2.442
Zn-S_{SH}	2.252	2.252	2.252
Angles (deg)			
H-C-H	110.1	110.1	110.0
P-O-C	123.4	123.2	122.2
S-P-O	112.7	111.6	110.5
O-C-H	108.8	108.8	108.9
O-P-O	97.9	101.3	104.9
S-P-S	108.2	109.2	110.2
S-Zn-S	85.0	85.1	95.5
Dihedral (deg)			
H-S-Zn-S	90	90	90
C-O-P-O	-179.7/-179.7	-179.6/57.9	66.6/66.6
Energy (kcal/mol)	0.13	0.00	1.19

Figure Captions

Figure 1S. Vibrational modes of the *tt* conformation for $[(MeO)_2PS_2]^-$ from HF LAV3P*** calculations. (a) PS antisymmetric stretch (PS_{anti}). (b) PS symmetric stretch (PS_{sym}).

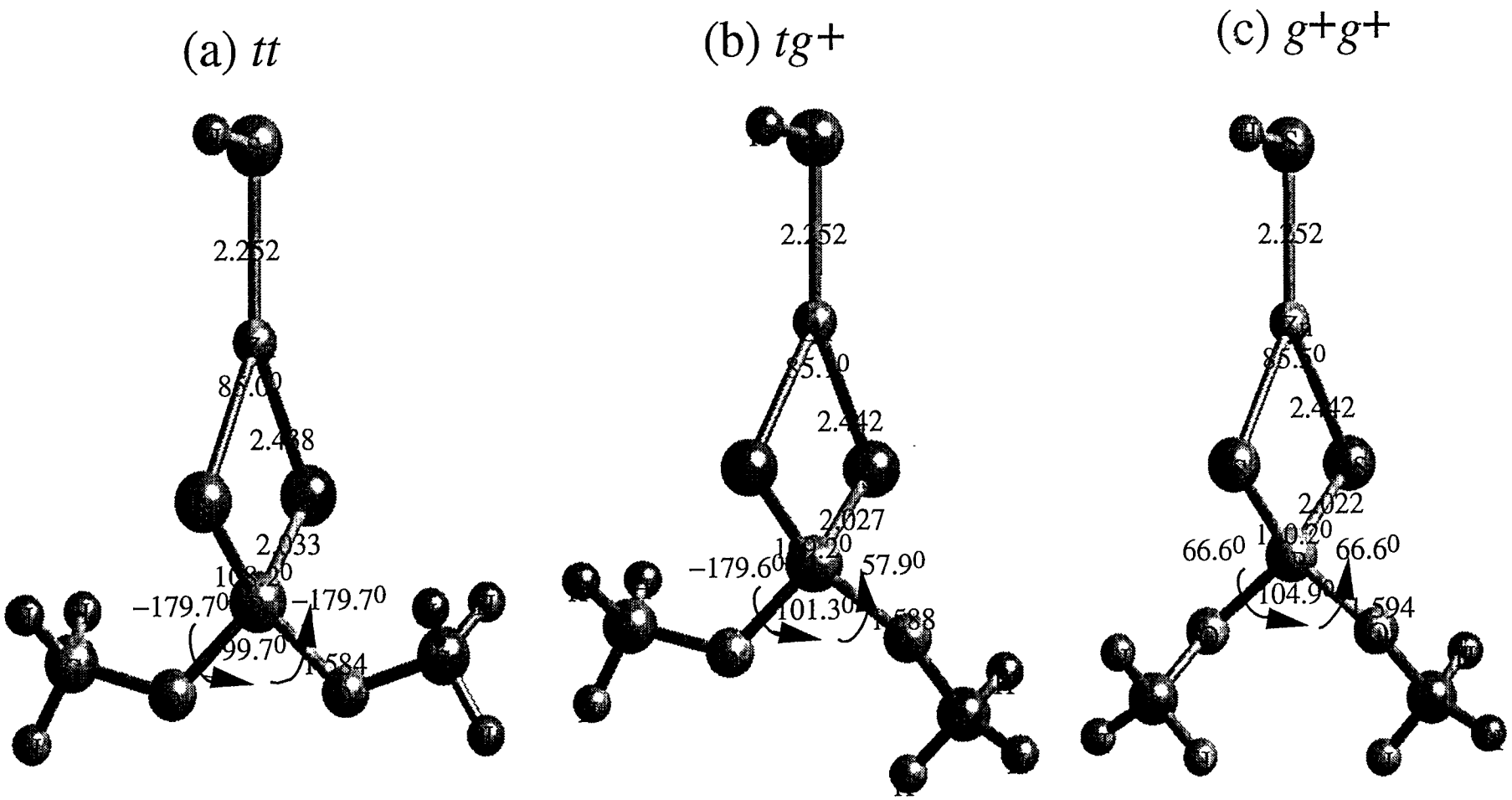

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Fig 4